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This report outlines the objective and the progress made in achieving some understanding of the difference solutions of complex flow problems in fluid mechanics, which are inevitably computed at rather coarse meshes. We developed a set of difference algorithms, analyzed them as to the behavior of the "errors" of the difference solutions of some model problems, and then applied them in the computational solution of the two dimensional

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interaction fields of a shock wave with a boundary layer, both for the laminar and for the turbulent cases with and without separation. The latest algorithm is developed specifically for computational solutions at coarse mesh attainable with a modest computer. We used mostly 1/4 capacity of the IBM 360-91 at Princeton University. It is shown how these solutions with comparable accuracy can be achieved with an order of magnitude reduction in computer time and capability when the new algorithm is used.

FINAL REPORT TO OFFICE OF NAVAL RESEARCH

Contract No. N 00014-75-C-0376

"The Application of Difference Methods in Fluid Mechanics"

The primary objective of the proposed research has been the development of difference methods for the solution of gas dynamic equations as a tool of fluid dynamics research and developmental work. Fundamental understanding is emphasized rather than the generation of specific solutions of various practical flow problems; although it has been conducted around two specific problems.

The first problem is the flow field of interaction of a shock wave with a planar boundary layer. The second problem is the supersonic flow over a yawed cone. The first problem is distinctly in two space dimensions while the second is dominated by important three dimensional effects.

The requirement of adequate resolution for the computational solution of 3D flow problems makes it necessary to consider the use of the very large and very high speed computers like the ASC or the STAR machines. The ASC computer was operational and available in 1977. In earlier years a certain amount of analysis was done and a preliminary computation was performed on the IBM 360-91 computer to learn about the various subtlties of the computational solution of the truely 3-D flows. We

began constructing the 3-D program for the computational solution of the yawed cone problem working on the ASC machine in 1977. We have low priority for our access to the ASC machine and have progressed by early 1978 only to the successful test of the unyawed configuration. It was decided in 1978 as was reported to the ONR office in Washington D.C. to devote our effort to the first problem in two space dimensions in the remaining period. Our schemes conceived earlier for generating the yawed cone solution from the axisymmetric situation was not tested on the ASC machine. A relatively complete picture is obtained for the first problem as a result.

From the preliminary studies of 3-D problems, the following "tentative conclusions" were obtained.

1. The stability of our computational algorithm is only slightly affected in the interior (of the field of computation). The ranges of Mesh Reynolds number for stable computations remains essentially unchanged, although the maximum amplitudes of oscillatory perturbations that permit stable computations can be significantly reduced at certain ranges of values of Mesh Reynolds numbers. The reduction of such maximal allowable disturbance amplitudes is really not harmful, since the lower limits of the amplitudes are too large to be tolerated in a reasonable solution anyway.

2. Proper treatment of the initial boundary conditions is considerably more critical in 3-D then in 2-D problems especially where shockwaves intersect the computational boundary. This aspect can be very important in the computational solution of such a complex problem as the supersonic flow over a yawed cone.

We have had no opportunity to try out in the full 3-D field any schemes of boundary treatment analyzed in model study.

It was decided to suspend the investigation of the yawed core problem in the spring of 1978, although certain analytic aspects of the yawed cone problem continued until fall. No concrete results can be reported. Partial documentation of the above results are contained in the two Master Theses by Sung and Specht and the incomplete manuscript of Mr. Grasso.

The treatment of the shock wave boundary layer interaction problem was divided into three stages:

1. Development of algrithms and their preliminary analysis and tests. The test computations include those for shock waves in one space dimension and then in two space dimensions.
2. Computational solution of the interaction field resulting from the incidence of a weak shock wave on a laminar boundary layer with and without separation.
3. Computational solution of the interaction field resulting from the incidence of a moderate shock on a turbulent boundary layer with separation.

It is generally presumed that by computing at sufficiently small meshes, the computed results would be"sufficiently accurate" although the errors may not be commeasurate with the local truncation errors. Such is true and proven for those linear, smooth, well posed problems. For those practical problems, which are nonlinear, not so smooth, and often poorly posed, this presumption is at best a plausible conjecture. This was discussed and exemplified quite extensively in the VKI lecture notes (1974)

by the author [4].

Our originial approach to the solution of the shock wave laminar boundary layer interaction problem was based on such conventional wisdom of successive mesh refinements; an approach which was apparently rather successful in our earlier investigation of similarly complex problems like near wake and leading edge flows. We did obtain very reasonable solutions (Ph.D. Thesis(Messina)), in much better agreement with experimental data than other available computational solutions.

The behavior of the successive iterates of Messina's solution raises however, some serious questions as was suggested by our linearized analysis of the phase errors in the solution. The oscillatory error components in the computed solution tends to be minimal when the phase of these oscillations change sign. Accordingly the error in the computational solution may reach a local minimum at some finite value of mesh Reynolds number. Mesh refinement beyond the critical value can cause deterioration of the computed solution.

The above preliminary result is amplified and confirmed by the detailed analysis of the system of nonlinear difference equations of one dimensional model equations. This analytic study (Ph.D. Thesis(Shubin)), confirmed the asymptotic nature of the convergence of the successive iterants with mesh refinements i.e. reducing the mesh Reynolds number. The convergence is likely to be non-uniform, especially when the difference formulation includes those extraneous boundary conditions commonly adopted in the solution of practical problems.

The errors in the computed solution may actually increase to fairly large values with further mesh refinements beyond the optimal limit. Whether the sequence of the iterants will eventually converge to the correct solution as $Re_{\Delta x} \to 0$ will depend on how well the difference problem is posed, whether the formulation is consistent and stable, and may be on other conditions. But it is apparent that when most common difference schemes are applied to complex practical problems, such a convergence region of sufficiently small $Re_{\Delta x}$ even if it exists, is well beyond the reach of computers in the forseeable future.

The analysis indicates further, that the magnitudes of the minimal error of the computed solutions at the critical mesh Reynolds number can be "comparable" to that of the convergent sequence at much smaller mesh Reynolds numbers.Thus, such computed solutions near the minimal errors at fairly large $Re_{\Delta x}$ may be as useful as the convergent approximations at much smaller $Re_{\Delta x}$. The situation is quite similar to the approximate evaluation of transcendental functions as the solutions of some ordinary differential equations. Such asymptotic approximations are then much more useful in practice than those convergent approximations.

When the class of simple difference algorithms which we analyzed (Shubin), is applied to complex practical problems in multi-space dimensions, there is an outstanding difficulty. The mesh Reynolds number generally varies over a much wider range of values in a complex flow problem than the plateau of errors around the critical mesh Reynolds number. Moreover, the stability of the complete difference formulation will depend

on the discretization parameter γ in the class of algorithm analyzed and there are indications of computational instability if γ is too large negatively. In order to take advantage of such asymptotic approximations of coarse mesh computational solution, we have to develope some algorithm that promises stable computation and small and very flat variations of errors at large mesh Reynolds numbers. This is accomplished by a simple modification of our two step algorithms .

Both the predictor and the correctors of the two step scheme of Cheng-Allen (Scheme 1) are defined over a single mesh (or grid) system. We now consider the predictor step defined on a sub-grid at mid-mesh points and let the function values at mid-mesh be the arithematic averages of the nearest neighbors. This new scheme (2) is obtained in a manner similar to Richtmyer's modification of the Lax-Wendroff scheme. Linearized analysis provides very encouraging signs as a scheme particularly suitable for coarse mesh computation. The scheme was further tested computationally with nonlinear Burgers' equation and then the Navier-Stokes equations in two space dimension for the simple flow field resulting from the deflection of a uniform supersonic stream by a straight oblique shock. The following encouraging results are obtained:

1. The maximal errors of the computed solution with scheme (2) is significantly below those with scheme (1) at large mesh Reynolds numbers ($Re_{\Delta x} \gtrsim 3$), although the reverse is true for $Re_{\Delta x} \lesssim 3$.

2. Over the entire range of $Re_{\Delta x}$ scheme 2 appears to provide

solutions well within the accuracy requirements ($\lesssim$ 10%) in engineering applications, and comparable to the accuracy of the data.

3. The oscillations (or rather overshoots) in results computed with scheme 2, if they should occur,are confined within a mesh or two away from the shock like discontinuity.

4. Scheme 2 converges to the "steady state" much faster than scheme 1, i.e. fewer number of steps are required to satisfy a given steady state criterion from a given initial state.

The same program for the Navier-Stokes equation is then used to solve the interaction field resulting from the incidence of a weak shock wave on a laminar boundary layer. In recognition of the nontrival pressure gradient along the wall and of the coarseness of our mesh, parabolic mean velocity profiles is used in the treatment of the wall cells. The cases to be calculated correspond to the experimental data of Hakkinen et. al. This unseparated case has been computationally solved by many authors including our solution by Messina with scheme 1, which represents the most "accurate" computational solution as judged by comparison with experimental data. Our interest is to demonstrate that with scheme 2, solutions as "accurate" as the above can be obtained at much coarser mesh, and with much less demand on computing time and computer capability. As is illustrated in the following table (see next page), our objectives are largely met with 1/8 of the number of grid points in the solution with scheme 2, the computer time required to reach steady state from the same initial data is reduced by a

TABLE II

Scheme	Mesh Size	Field Size (IE x JE)	Core (K bytes)	Cycle Time (sec/cycle)	No. of Time Steps	CPU (min : sec)
1 (Messina)	$\Delta x = 4\Delta y$	53 x 117	362	1.38	1200	27:36
	$\Delta x = 2\Delta y$	53 x 233	580	2.77	900	41:33
					TOTAL CPU	69:09
2 (Present)	$\Delta x = 8\Delta y$	27 x 30	200 Program ~175 Data Storage ~25	0.218	600	2:11

factor 1/30. The 200 K-bytes of the computer storage required is largely to accomodate the program (175 K-bytes), which, if streamlined, can be substantially reduced. Thus a problem of comparable complexity can be handled with computers with a fraction of the capabilities of the IBM 360-91. Using IBM 360-91 it is possible to compute somewhat more complex problems.

The separated case of Hakkinen's data was not successfully computed with scheme 1, possibly because of poor stability and/or slow convergence toward steady state. This case is now solved with scheme 2 at half the mesh size; and the steady state criterion was satisfied after 1200 cycles (vs. 600 for unseparated case) and 15 minutes (v.s. 2.4 minutes) of computation with IBM 360-91. The results compare as favorable with experimental data as are the unseparated case. The separation bubble is very substantial, which makes it necessary to extend the field of computation to $76\delta_1$ compared with $58\delta_1$ for the unseparated case.

The successful completion of the separated case of shock-wave laminar boundary layer interaction encourages us to obtain computational solution of similar interaction problem with turbulent boundary layer. There remains two outstanding problems. The first one is physical that a model for the turbulence stress is needed. The second one is computational since it is as yet uncertain whether scheme 2 at coarse mesh can successfully handle the "intersecting shockwaves" i.e. the incident shock and the induced shock wave sprang from the "sudden" response of the turbulent boundary layer to downstream

pressure rise.

To focus our attention on the computational aspects of the problem, we decided to adopt an eddy diffusivity model of turbulent stress so that the governing differential equations system will still be the Navier-Stokes. The eddy diffusivity ε is chosen algebraically so as to represent the stress variation across the turbulent boundary layer properly. Thus in the outer region ε is specified according to clauser, and in the inner wall region to the model of Townsend and Mellor. Since separation is present in the case to be calculated, the wall model was extended further to include separation and separated layers.

Computational solutions were then attempted for the following cases in a Mach 3 supersonic stream with shocks, giving the flow deflection angles $\theta = 7.93°$, $9.87°$ and $10.83°$, incident on a turbulent boundary layer with $Re_{\delta 1} \simeq 1.5 \times 10^5$. The cases correspond to the experimental data of Law and have also been solved computationally by Shank et.al. Shank et.al. employed a slightly different eddy diffusivity model and introduced a relaxation parameter λ which was adjusted to achieve fit with known experimental results of Law. The present results for these cases agree with Law's experimental data as well but without the adjustable relaxation parameter. All cases involve some region of separated flow.

One more case with $\theta = 12.75$ at $Re_{\delta 1} = 2.5 \times 10^5$ was computed. It corresponds to the experimental data of Bogdonoff and Kepler. This case contains the largest separated region.

TABLE III

Method	Algorithm Employed	Computer Used	Computer Storage or No. of Grid Points	Computing Time	Mesh Configuration	Computed Case
Saffman-Wilcox Turbulence Model (Ref. 16)	AFTON von Neumann & Richtmyer	CDC7600	3885 Grid Points	2.71 Hours	Mesh Stretching in Y-Direction	$M_1 = 3$ $Re_{\delta 1} = 2.5 \times 10^5$ $\theta = 12.75°$
Eddy Viscosity with Relaxation Parameters (Ref. 17)	Mac Cormack Algorithm with Smoothing	CDC6600	Full use of Memory Core ~800 to 1000 Kbyts	About 2 Hours	"	$M_1 = 3$ $Re_{\delta 1} = 1.5 \times 10$ $\theta = 12.27°$
Eddy Viscosity and Wall-Layer Turbulence Model (Present)	<u>Scheme 2</u>	IBM 360/91	250K bytes or About one-fourth of Full Memory Core	About 1/2 Hour	Constant Mesh	$M_1 = 3$ $Re_{\delta 1} = 2.5 \times 10$ $\theta = 12.75°$

A table illustrating computer requirements of various different methods employed to calculate TBL-shock interaction problem.

It has been computed by Wilcox based on Saffman's differential model of turbulence. The present results with eddy diffusivity compares more favorably with the experimental data. There is clearly room for improvement especially quantitatively; but the computed results appear quite satisfactory. It is not possible to identify how much of the existing disparity between the experimental data and the computed results is due to errors in the computational procedure and/or those in the turbulence model. We are particularly encouraged by the fact that our coarse mesh scheme can compute successfully the configuration of intersecting shocks as well as the abrupt generation of a shock wave from the sudden changes in the turbulent boundary layer. Both the two shock and the three shock interaction configuration have been successfully computed. The use of coarse mesh and the relatively fast convergence with the present scheme 2 permits significant savings in computer time. This is illustrated in the following Table.

In conclusion, we have developed a new difference scheme (scheme 2) particularly suited for the computational solution of complex flow problems with rather coarse mesh. The various examples of the computational solution of the interaction field resulting from the incidence of a shock wave on a boundary layer with or without separation, laminary or turbulent, are probably as complex as many problems of practical interest. The new scheme is simple and convenient to use. It possesses good stability property and appears to converge toward the "steady state" considerably faster than our earlier scheme 1. It is

particularly suitable for coarse mesh computations. All these factors contribute to significant savings in computer time. Moreover, it opens up the possibility of the computational solution of rather complex flow problems with modest computer requirements. We have thus reached a definite stage of developing difference methods for the solution of gas dynamic equations as a tool of fluid dynamics research and development. Details of the development and test of the new algorithms are largely contained in the Ph.D. thesis of L. Oey. Technical reports are being prepared for submission for Journal publication. They will be distributed according to the ONR distribution list when published.

Documentation Generated

Journal Publications

During the contractural period 1972 - 1979, the following technical publications have been generated, or are under preparation.

1. "Finite Difference Treatment of Strong Shock over a sharp Leading Edge with Navier-Stokes Equations". (with J.H. Chen), Proceedings of 3rd International Conference on Numerical Methods in Fluid Mechanics., Paris (1972), Published in Lecture Notes in Physics Series No. 18 (1973), Springer Verlag.

2. "Friction and Heat Transfer Laws in Slip Flows", Proceedings in 10th International Symposium on Space Technology and Science, Tokyo, Japan 1973.

3. "Slip Friction and Heat Transfer Laws in a Merged Region" (with J.H. Chen), The Physics of Fluid, Vol, 17, No. 9 (1974).

4. "A Critical Review of Numerical Solutions of Navier-Stokes Equations", Lecture series delivered at Von Nauman Institute of Aerodynamics, Belgium, 1974. Published in "Progress in Numerical Fluid Dynamics", Edited by H.J. Wirz, Lecture note in Physics series No. 41 (1975) Springer Verlag.

5. "Computational Accuracy and Mesh Reynolds Number", (with .G. Shubin), Journal of Computational Physics 28 (1978).

6. "One Dimensional Gas Dynamics Model Study of Computational Accuracy" (.G. Shubin), accepted to appear in Journal of Computational Physics.

7. "Errors in Finite Difference Solutions of Navier-Stokes Equations", Proceedings of 6th International Conference on Numerical Methods in Fluid Mechanics. Tbilis U.S.S.R. (1978) to be published in Lecture Notes in Physics Series.

8. "Coarse Mesh Computational Solution of Navier-Stokes Equations", (with L. Oey) in preparation, to be submitted for Journal publication.

9. "Interaction of Shock Wave with Laminar Boundary Layer" to be prepared with (N. Messina and L. Oey).

10. "Computational Solution of the Interaction of a Shock Wave with a Turbulent Boundary Layer", to be prepared with (L. Oey).

University Reports

Ph.D. Thesis

1. J.H. Chen, "Finite Difference Methods and the Leading Edge Problem", 1971.

2. N.A. Messina, "A Computational Investigation of Shock Waves, Laminar Boundary Layers and their Mutual Interaction", 1977.

3. G.R. Shubin, "One Dimensional Gas Dyanmic Modeling and Computational Accuracy", 1977.

4. L.Y. Oey, "Large Mesh Reynolds Number Computations - with Applications to Shock Boundary Layer Interaction Problems", 1979.

5. K. Meintjes, in preparation, expected 1979 (tentative title - "Predictor-Corrector Methods for Time Dependent Compressible Flows").

6. F. Grasso, "Computational Solution of Supersonic Flow over a Yawed Core". (incomplete).

M.S.E. Thesis

1. T.C. Sung, "Numerical Solution of Partial Differential Equations with Various Formulations of Boundary Conditions" 1975.

2. R.C. Specht, "A Study of Computational Solution of Burgers' Model in Multispace Dimensions", 1977.